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Adaptive spectral tensor-train decomposition for the construction of surrogate models

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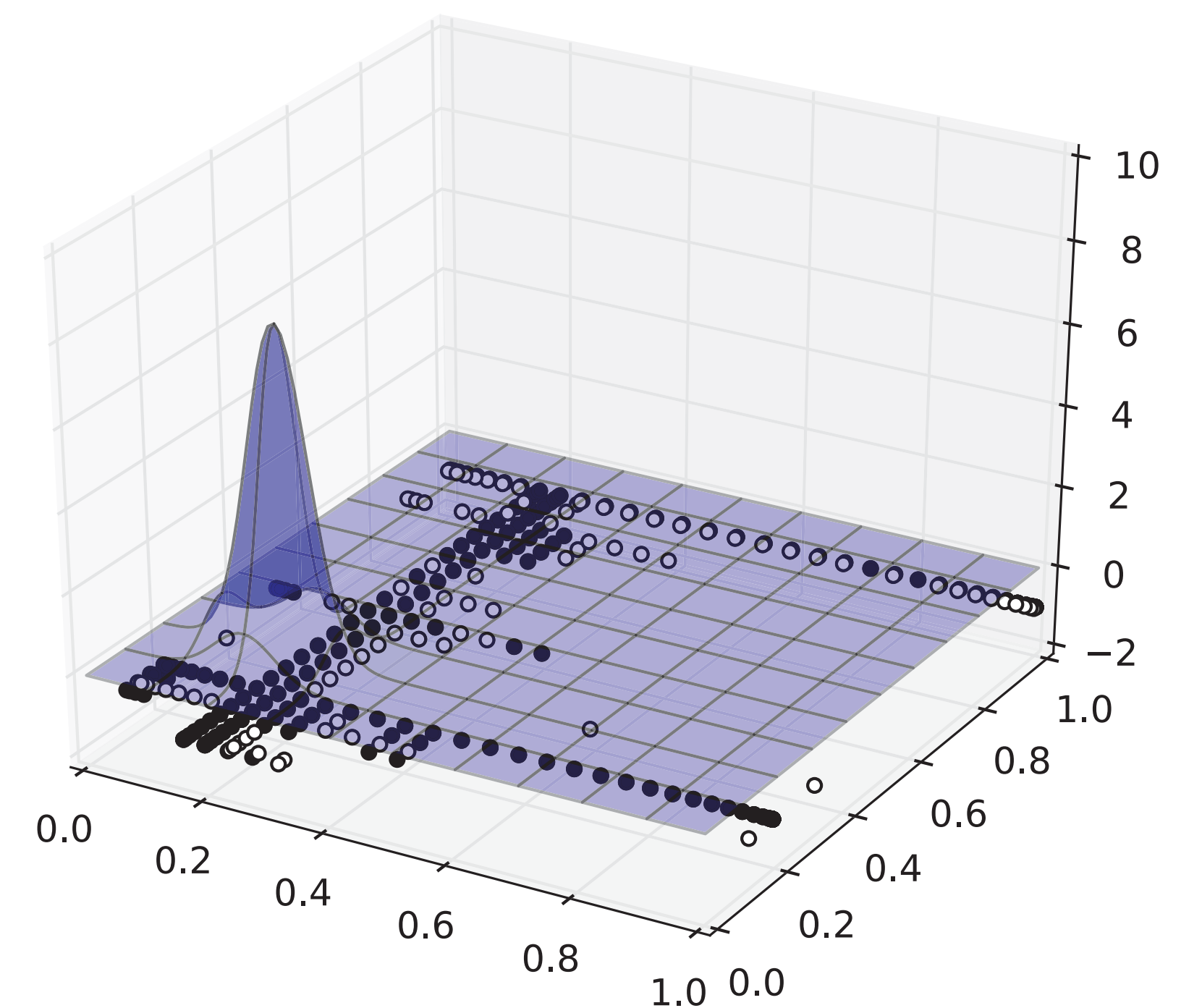
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PyPI: <https://pypi.python.org/pypi/TensorToolbox/> (LGPLv3)

⌚: <http://www2.compute.dtu.dk/~dabi/>

Introduction

The construction of surrogate models is important as a mean of acceleration in computational methods for uncertainty quantification (UQ). When the forward model is particularly expensive, surrogate models can be used for the forward propagation of uncertainty [4] and the solution of inference problems [5]. An adaptive construction is necessary to meet the prescribed accuracy tolerances with the lowest computational effort.



Problem setting

We consider $f \in L^2_\mu([a, b]^d)$, $d \gg 1$, and $\mathbf{x} \in [a, b]^d$ to be the variables entering the formulation of a parametric problem.

When to construct a surrogate?

- f is computationally expensive
- f needs to be evaluated many times
- the construction complexity pays off

Spectral tensor-train

Functional tensor-train approximation [1]

For $\mathbf{r} = (1, r_1, \dots, r_{d-1}, 1)$, let f_{TT} be s.t.

$$f_{TT} = \arg \min_{g \in L^2_\mu} \|f - g\|_{L^2_\mu}$$

$$g(\mathbf{x}) = \sum_{\alpha_0, \dots, \alpha_d=1}^{\mathbf{r}} \gamma_1(\alpha_0, x_1, \alpha_1) \cdots \gamma_d(\alpha_{d-1}, x_d, \alpha_d)$$

where $\langle \gamma_k(i, \cdot, m), \gamma_k(i, \cdot, n) \rangle_{L^2_\mu} = \delta_{mn}$.

FTT-approximation convergence [1]

For $f \in \mathcal{H}^k_\mu$, $k > d - 1$ and $R_{TT} = f - f_{TT}$,

$$\lim_{r \rightarrow \infty} \|R_{TT}\|_{L^2_\mu} = 0$$

FTT-decomposition and Sobolev spaces [1]

Let $\mathbf{I} \subset \mathbb{R}^d$ be closed and bounded, and $f \in L^2_\mu(\mathbf{I})$ be a Hölder continuous function with exponent $> 1/2$ such that $f \in \mathcal{H}^k_\mu(\mathbf{I})$. Then f_{TT} is such that $\gamma_j(\alpha_{j-1}, \cdot, \alpha_j) \in \mathcal{H}^k_{\mu_j}(I_j)$ for all j , α_{j-1} and α_j .

Let $P_N : L^2_\mu(\mathbf{I}) \rightarrow \text{span}(\{\Phi_i\}_{i=0}^N)$ where $\{\Phi_i\}_{i=0}^N$ are orthogonal polynomials:

STT-Projection

$$P_N f_{TT} = \sum_{i=0}^N c_i \Phi_i$$

$$c_i = \sum_{\alpha_0, \dots, \alpha_d=1}^{\mathbf{r}} \beta_1(\alpha_0, i_1, \alpha_1) \cdots \beta_d(\alpha_{d-1}, i_d, \alpha_d)$$

$$\beta_n(\alpha_{n-1}, i_n, \alpha_n) = \int_{I_n} \gamma_n(\alpha_{n-1}, x_n, \alpha_n) \phi_{i_n}(x_n) \mu_n(dx_n)$$

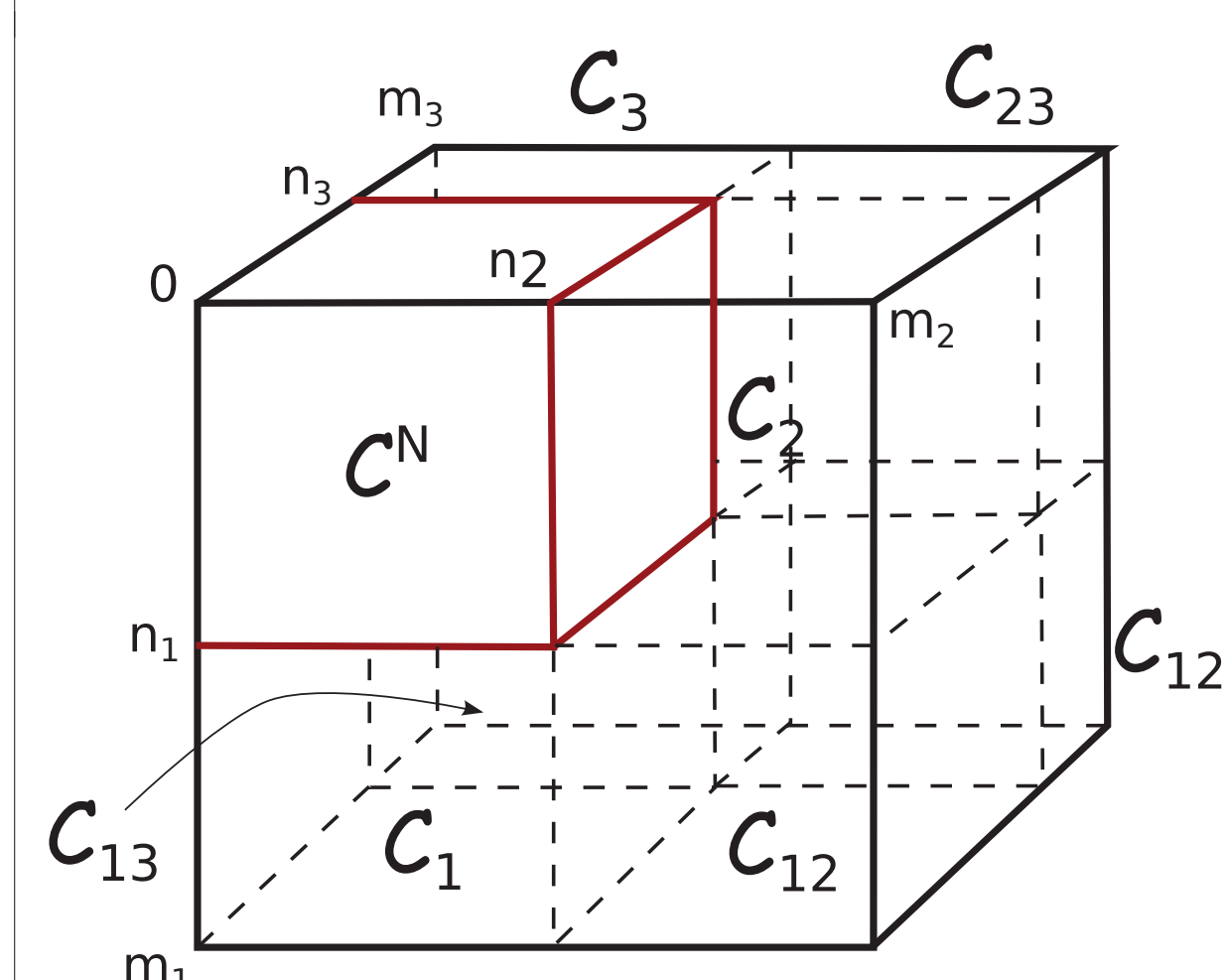
STT-Projection convergence

Let $f \in \mathcal{H}^k_\mu(\mathbf{I})$, then

$$\|f - P_N f_{TT}\|_{L^2_\mu} \leq D(k) r^{-\frac{k+1-d}{2}} \|f\|_{\mathcal{H}^k_\mu} + C(k) N^{-k} |f_{TT}|_{\mu, k}$$

The construction is performed using the tensor-train decomposition [6] of tensorized quadrature rules, obtained through the deterministic sampling algorithm TT-dmrg-cross [7], achieving scalable $\mathcal{O}(dNr^2)$ complexity.

Anisotropic adaptivity

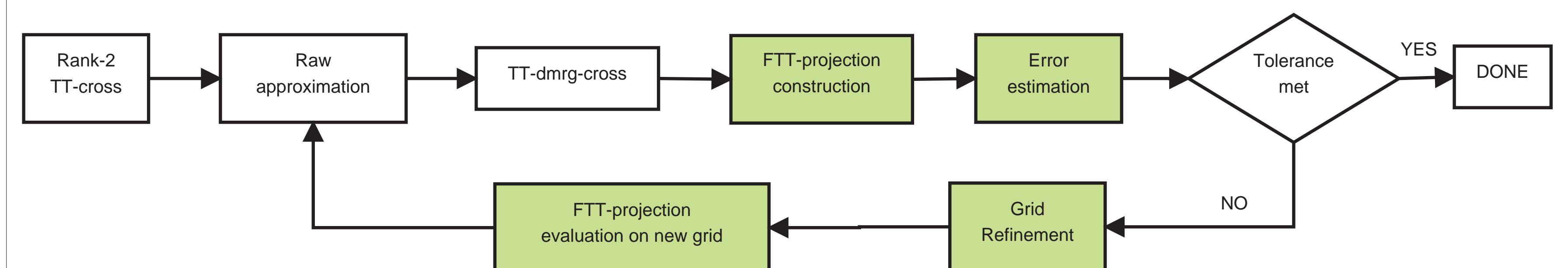


Let $\mathbf{N} = (n_1, \dots, n_{d_s})$ and $\mathbf{M} = (m_1, \dots, m_{d_s})$ s.t. $\mathbf{N} < \mathbf{M}$. Then

$$\|P_N f_{TT} - P_M f_{TT}\|_{L^2_\mu} = \sqrt{\sum_{i=N}^M c_i^2} = \sqrt{\sum_{i=1}^M \|\mathbf{c}_i\|_F^2 + \sum_{i=2}^M \|\mathbf{c}_i\|_F^2 + \cdots}$$

Let us define the n -th order error contribution in the j -th direction:

$$\mathcal{E}_j^{(n)} = \left(\|\mathbf{c}_j\|_F^2 + \sum_{i=2}^n \|\mathbf{c}_i\|_F^2 + \cdots + \sum_{i=n}^M \|\mathbf{c}_i\|_F^2 \right)^{\frac{1}{2}}$$



Numerical experiments – Modified Genz functions

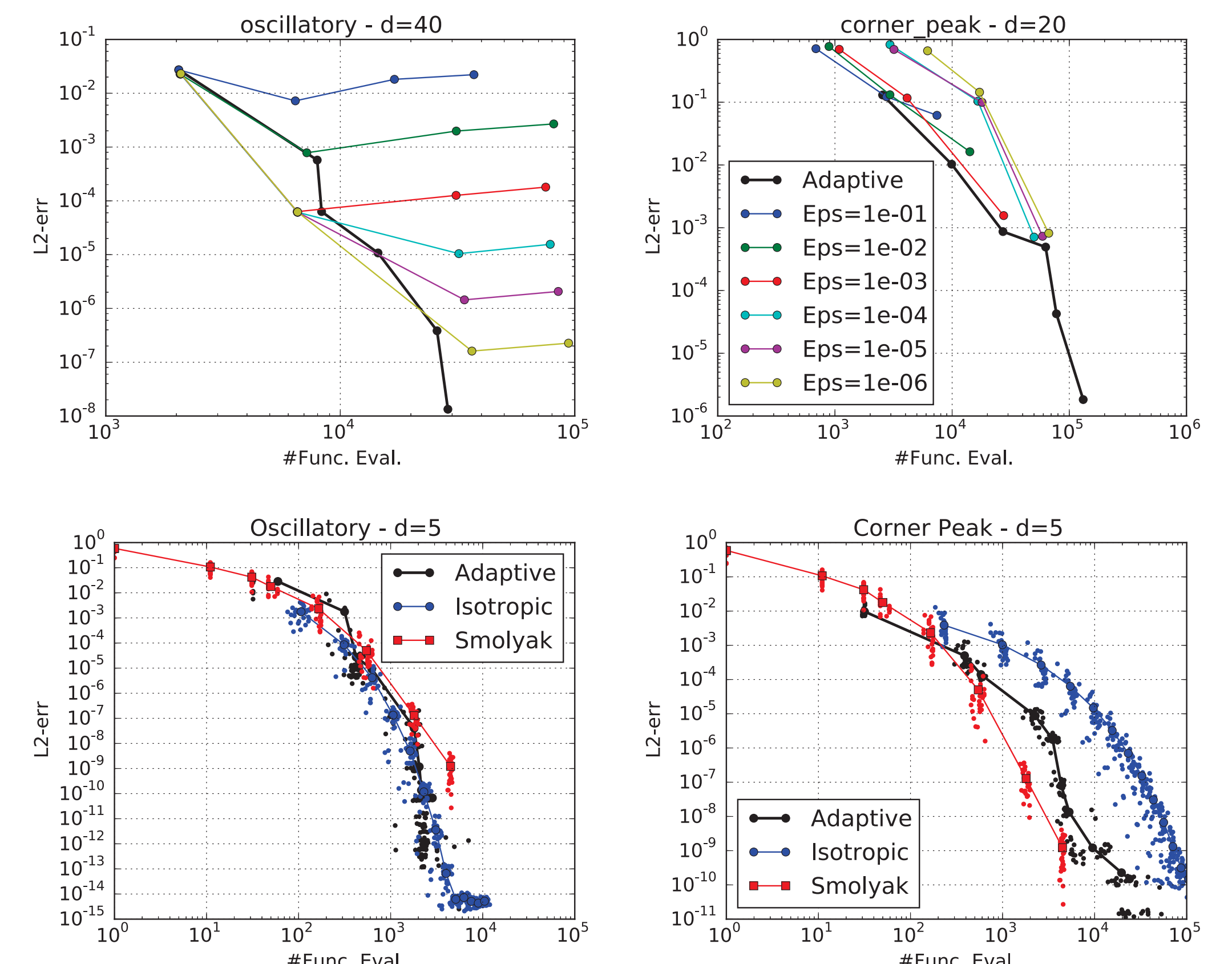
Oscillatory : $f_1(\mathbf{x}) = \cos\left(\sum_{i=1}^d 2^{c_i} x_i\right)$

Corner Peak : $f_2(\mathbf{x}) = \left(1 + \sum_{i=1}^d 2^{c_i} x_i\right)^{-(d+1)}$

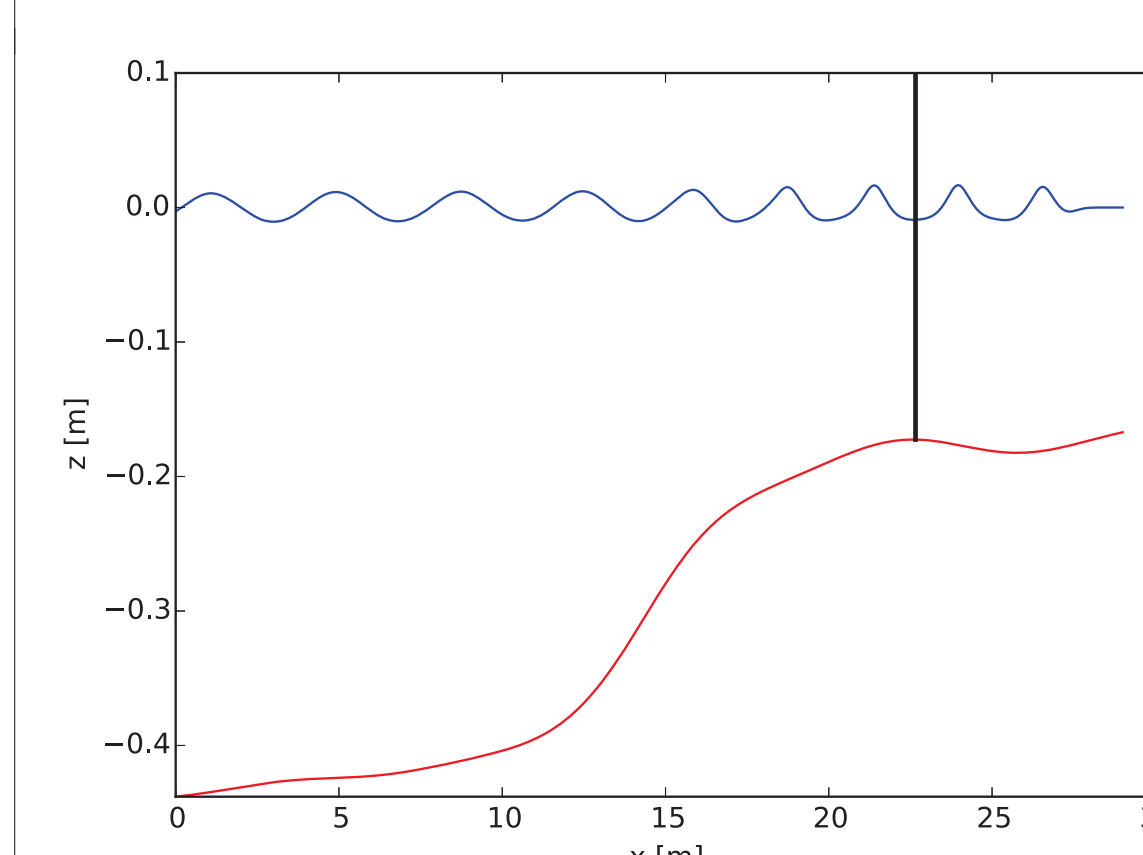
$$c_i \sim \begin{cases} Be(2, 8) & \text{if } p_i < 0.5 \\ Be(8, 2) & \text{otherwise} \end{cases}$$

$p_i \sim \text{Bernoulli}(0.5)$

The performances are evaluated on the Genz functions up to $d = 100$, and compared to the results obtained with the anisotropic Smolyak pseudo-spectral approximation [2]. The adaptivity avoids over-fitting and under-fitting due to discrepancy between the polynomial order and the FTT tolerance.



Uncertain wave loads on offshore monopiles



Scalable flexible-order finite difference of nonlinear and dispersive potential flow [3] for shoaling water waves subject to uncertain bathymetry ($d = 10$).

ε	N.f.e.	$L^2\text{-err}$	$E[\text{Load}]$
5×10^{-1}	221	3.8×10^{-2}	$9.962 \times 10^{-2} N$
1×10^{-1}	236	2.4×10^{-2}	$9.866 \times 10^{-2} N$
5×10^{-2}	260	7.3×10^{-3}	$9.766 \times 10^{-2} N$

Features

- Linear scaling w.r.t. d
- Incremental construction
- Storage and re-starting
- Parallel implementation

Outlook

- Investigation of nested rules
- UQ on 3D water waves [3] interaction with structures

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